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(54) Title: SELF-GUIDED MOLECULAR DYNAMICS SIMULATION FOR EFFICIENT CONFORMATIONAL SEARCH

(57) Abstract

A method of forming a generated conformation of a molecular system comprising generating a molecular dynamics trajectory of said molecular system, wherein said trajectory is initiated by assigning to each atom in said molecular system a set of initial parameters comprising an initial velocity vector and an initial conformation wherein each atom in said molecular system is disposed in an initial position, and wherein said molecular dynamics trajectory is propagated by a computational procedure comprising: (a) calculating a current force exerted on each atom (i) by calculating a derivative of an energy function describing interactions between said atom (i) and other atoms in said molecule; (b) determining a guiding force g_i describing an average along a portion of said trajectory of a force exerted on said atom (i); (c) determining a current position and velocity of said atom (i) by ajusting said previous position and velocity according to the equation $m_i a_i = f_i$, wherein m_i is the mass of atom (i), a_i is an acceleration of atom (i) and f_i is a force obtained by adding said current force calculated in (a) and said guiding force determined in (b); (d) replacing said previous position and velocity of said atom (i) with said current position and velocity of said atom (i); (e) repeating steps (a) to (d) for one or more iterations to generate said trajectory; and (f) forming said generated conformation by disposing the atoms of said molecule in respective current positions obtained during a given iteration; and processing said generated conformation to determine a structural, energetic, thermodynamic or kinetic property of said molecular system.